The AMP Nuclear Fuel Simulation Code

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In one year, a multi-lab collaboration has produced a new 3D scalable parallel nuclear fuel performance simulation code within the DOE Office of Nuclear Energy NEAMS program, which aims to provide high-fidelity simulations to accelerate the development of new nuclear reactor fuel designs. Processes such as fission heat generation and thermal transport, fission product generation and chemical transport, mechanics with elasticity, plasticity, swelling, densification, and thermal- and irradiation-induced creep, and surface interactions between the pellet, cladding, and coolant are modeled. Existing scalable parallel solver software from other DOE programs and laboratories was highly leveraged. Initial results compare favorably with experimental data and legacy simulations.

With an increased national emphasis in recent years on developing carbon-neutral energy sources, nuclear power has enjoyed revived interest. However, significant expansion of the existing fleet of commercial thermal-spectrum light-water reactors (LWR) is unattractive due to concerns about waste disposal and diversion, caused by significant amounts of unburned fissionable fuel at the end of the useful life of fuel rods. Mechanical failure of the rods occurs long before the fissionable elements are consumed from radiation-induced swelling, creep, fracture, hydriding, etc. Development of advanced reactors with a fast neutron spectrum for high burnup can address the waste concerns, but there are significant barriers to their development. It just is not currently known how to design materials and equipment to survive the enhanced radiation load generated in such a reactor. The traditional experimental method (sometimes called “cook and look”) of constructing a test article, inserting it into a reactor for a period of months or years, and examining it afterward in a hot cell is expensive and time-consuming. To accelerate the development of advanced reactor materials and designs the Department of Energy (DOE), based on the success of its Advanced Simulation and Computing (ASC) and Scientific Discovery through Advanced Computing (SciDAC) programs, has launched the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program [1], which seeks to develop Integrated Performance and Safety Codes (IPSC) for fuels, reactors, actinide separations, and waste forms and disposition. These codes are targeted to add computational insight to experimental insight in order to transform the design of critical components such as fuel pins, reactor vessels, liquid centrifugal contactors, and repositories. They will integrate knowledge at all scales, from the atomistic level to an entire plant, and take advantage of the latest DOE computing platforms.

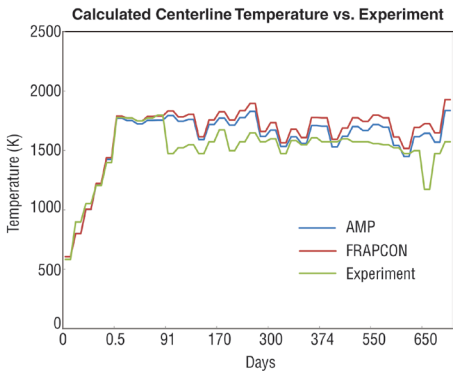

Fig. 1. Centerline temperatures for FRAPCON, AMP, and experimental data for Halden IFA432 rod 1 over 759 days.

The NEAMS fuels IPSC is called AMP, and has been under intensive development for about a year by a collaboration of personnel from ORNL, LANL, and INL. Nuclear fuel evolution is governed by a complex interplay of physical processes at multiple coupled-length scales. A fuel rod generally consists of a steel or zirconium alloy tube (cladding) a few meters long enclosing a stack of cylindrical fuel pellets about a centimeter across and a centimeter tall. In the fuel pellet, nuclear fissions generate heat, product nuclei, and a wide variety of materials-damage phenomena. At the engineering scale, the AMP code must model fission heat generation and thermal transport, fission product generation and chemical transport, mechanics with elasticity, plasticity, relocation, swelling, densification, and thermal- and irradiation-induced creep, and surface interactions between the pellet, cladding, and coolant. The first release of the AMP code, available through the Radiation Safety Information Computational Center at ORNL [2], models all of these processes in 3D. The code makes extensive use of scalable parallel numerical solver software packages developed by the DOE over the years, such as TRILINOS (SNL), PETSc (ANL), and SUNDIALS (LLNL), seamlessly integrated by an ORNL-developed computational backplane.

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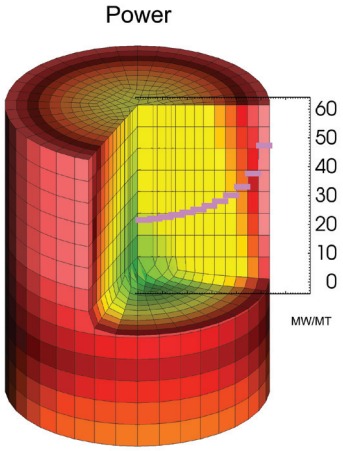


Fig. 2. Modified 3D power distribution in pellet with radial rim effect and axial peaking.

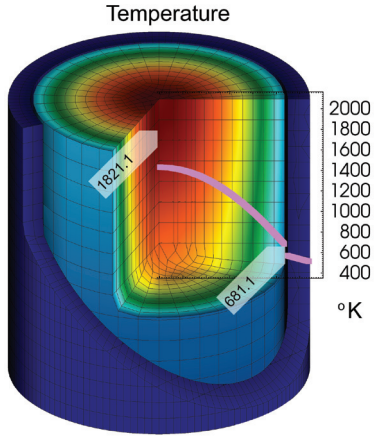
For fuel performance simulation, many material properties, such as nuclear cross sections, transport coefficients, and mechanical response, must be modeled. A few models exist for these properties, developed over the years through the "cook and look" approach, that are being incorporated into AMP, but for the NEAMS program to succeed they must be extended in range to regimes where experimental data is difficult to obtain in a timely manner. Accordingly, NEAMS is employing a variety of lower-length-scale codes to provide some of these properties computationally. For example, the INL phase-field code MARMOT will provide meso-scale property evaluations using data from atomistic simulations performed with the LANL SPaSM code.

There are deep ties between the AMP project and other components of the DOE Office of Nuclear Energy due to common interests and personnel. Experimental data for AMP material models and validation will be provided by the Fuel Cycle Research and Development (FCRD) program [2], and AMP will provide nuclear fuel modeling capability to the Consortium for Advanced Simulation of Light water reactors (CASL) energy innovation hub [3].

For the AMP code, ADTSC personnel developed the thermal and chemical transport component (Gary Dilts, CCS-2) and provided program development and management (Cetin Unal, CCS-DO). In addition, former ADTSC personnel now at ORNL are heavily involved (John Turner, CCS-2, and Bobby Philip, T-5). The material properties library was jointly developed by Gary Dilts and Bogdan Mihaila (MST-6), and Mike Rogers (XCP-8) performed verification testing. A team led by Chris Stanek (MST-8) is performing atomistic simulations.

The principal legacy fuel performance simulation code is FRAPCON from PNNL. The IFA432 test assembly was irradiated at the Halden reactor in Norway with a complex power history from 1975 to 1984, and provides FRAPCON validation data [4]. Figure 1 shows a comparison of experimental centerline temperatures, AMP 3D simulation results, and FRAPCON 1D results over a period of 759 days. The AMP results follow the FRAPCON results fairly well. Figure 2 shows a hypothetical 3D perturbation of the power distribution in a pellet for the validation problem used in Fig. 1. The radial rim effect and axial peaking were modeled. Figure 3 shows the resulting 3D temperature distribution in a single fuel pellet with its surrounding cladding, which represents just a small section of a fuel rod (for more information see [5]).

Fig. 3. Three-dimensional temperature distribution calculated by AMP using power distribution of Figure 2 at 20th burnup step.



[1] NEAMS, http://www.ne.doe.gov/AdvModelingSimulation/program.html
[2] RSICC (Radiation Safety Information Computational Center) http://www-rsicc.ornl.gov
[2] FCRD, http://www.ne.doe.gov/fuelcycle/neFuelCycle.html
[3] CASL, http://www.casl.gov
[4] Lanning D.D., et al, "FRAPCON 3 Integral Assessment," NUREG/CR-6534, PNNL (YEAR).
[5] Dilts G., et al., "The AMP (Advanced MultiPhysics) Nuclear Fuel Integrated Performance and Safety Code," LA-UR-10-07059 (2010).

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